Simulations of an Ar/HBr microwave source etch process and the effect of SiBr and SiBr2 cross-sections.

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63rd GEC & 7th ICRP, QR2_2
Thurs. 7th Oct. '10, 16:30
Global Model

Electron Chemistry

Data

Reactors Model

Data

Informs

Validates

Process and Tool Development

Measurement, Experimentation
Modeling polyatomic electron-molecule interactions

What does Quantemol-N do?

- Elastic cross sections
- Electronic excitation cross sections
- Electron impact dissociation
- Rates
- Resonance parameters
- Eigenphase sums
- Ionisation cross sections
- Dissociative electron attachment
- Differential cross sections
- Momentum transfer cross sections
- Vibrational excitation cross sections

How does Quanitemol-N work?

The R-Matrix Method

- The sphere, of radius $a$, has the centre of mass of the molecule as its origin;
- the sphere contains the electron cloud of the molecule;
- equations of motion are solved in the body-fixed frame (fixed nuclei approximation)

### Progress...

<table>
<thead>
<tr>
<th>CF2</th>
<th>C6H6</th>
<th>C5H12</th>
<th>SiH4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cl2</td>
<td>C3H4</td>
<td>NO2</td>
<td>C2H6</td>
</tr>
<tr>
<td>O2</td>
<td>C2</td>
<td>NO</td>
<td>C3H8</td>
</tr>
<tr>
<td>H2O</td>
<td>C3H6</td>
<td>O3</td>
<td>HCN</td>
</tr>
<tr>
<td>H3+</td>
<td>CaF+</td>
<td>PH3</td>
<td>HNC</td>
</tr>
<tr>
<td>CH4</td>
<td>CaF</td>
<td>BF3</td>
<td>SiO</td>
</tr>
<tr>
<td>C3N</td>
<td>CF</td>
<td>N2</td>
<td>CS</td>
</tr>
<tr>
<td>Cl2O</td>
<td>CO2</td>
<td>CO</td>
<td>F2</td>
</tr>
<tr>
<td>CONH3</td>
<td>BF3</td>
<td>H2</td>
<td>HBr</td>
</tr>
</tbody>
</table>

... and more.
CF$_4$/O$_2$ CCP etch

0-D plasma simulation

CCP etching chamber

SCCM
RLSA (Radial Line Slot Antenna) micro-wave plasma reactor

1. Micro-wave excited a high density plasma.
2. Plasma is transported by diffusion, Te is cooled and uniformed.
3. RF bias works only accelerating ion, not for plasma generation.
Why does High Press. Process make vertical profile?

**Pressure dependency**

HBr/Ar Process
Vpp : Const. = 415V
Residence time : Const. = It is proportional to Pressure

<table>
<thead>
<tr>
<th>Press.</th>
<th>40mT</th>
<th>70mT</th>
<th>80mT</th>
<th>100mT</th>
</tr>
</thead>
<tbody>
<tr>
<td>RF</td>
<td>113W</td>
<td>80W</td>
<td>73W</td>
<td>70W</td>
</tr>
<tr>
<td>Etch.D</td>
<td>232(147%) / 158</td>
<td>205(144%) / 142</td>
<td>204(121%) / 168</td>
<td>216(108%) / 200</td>
</tr>
<tr>
<td>Taper</td>
<td>81· / 68·</td>
<td>86· / 81·</td>
<td>86· / 84·</td>
<td>86 / 85·</td>
</tr>
</tbody>
</table>

The higher pressure, The Dense/Iso pattern dependence is getting better
Reaction model

-Charged species: e\textsuperscript{−}, Br\textsuperscript{−}, Ar\textsuperscript{+}, HBr\textsuperscript{+}, Br\textsuperscript{+}, Br\textsubscript{2}\textsuperscript{+}, SiBr\textsubscript{2}\textsuperscript{+}, and SiBr\textsuperscript{+}

-Neutral species: Ar, Ar\textsuperscript{*}, HBr, Br, Br\textsubscript{2}, H\textsubscript{2}, H, SiBr\textsubscript{2}, SiBr, and Si

-Electron impact reactions: Ionization, excitation, dissociation, attachment, and recombination

-Ion – neutral reactions

-Ion – ion reactions

-Molecule – molecule reactions

SiBr\textsubscript{2}+, SiBr\textsuperscript{+}, SiBr, and Si are omitted in case without SiBr\textsubscript{x} reactions.
SiBr
49 Electrons

Bond length: 2.641 Ang.
$e + \text{SiBr}$

Cross-section (ang. sqrd.) vs. Energy (eV)

- Ionisation
- Elastic
- Dissociative impact
- Dissociative Attachment
SiBr$_2$
84 Electrons

Bond length: 2.039 Ang.
Bond Angle: 122.8 Deg.
e + SiBr2 >

- Elastic
- Dissociative impact
- Dissociative Attachment
- Ionisation

Energy (eV) vs. Cross-section (ang. sqrd.)
Surface reactions with Walls

- Open
- $\text{Br}_2$
- HBr
- H
- Br
- H
- H
- HBr
- Br
- $\text{H}_2$
Surface reactions with wafer

\[ ER / \rho = s_i \Gamma_i (\theta_{SiBr} + \theta_{SiBr_2}) \left( \Gamma_{Si} + \Gamma_{SiBr} + \Gamma_{SiBr_2} \right) \theta_{Si} - \left( \Gamma_{Si} + \Gamma_{SiBr} \right) \theta_{SiBr} \]
Simulation model

- Comsol
- Gas flow
- Electron temperature
- Charged particles
- Neutral particles

Jozef Brcka, Song-Yun Kang,
Microwave

Wafer

Stage with rf bias

Gas flow

Gases inlet

Pumping out

Gas flow
Electron distributions are localized near top, because microwave heat comes from top.
Br negative ion produced both inlet and near wafer because of attachment reaction of SiBrx.
SiBr2 in case with SiBrx reactions is localized near wafer because there are reactions of SiBr2.
SiBr and Si are produced from SiBr2 and SiBr respectively.

Ions produced from byproducts are localized near wafer which is dominant ions attack to wafer.
Ion fluxes on wafer

Without SiBrx reactions

Including SiBrx reactions
Ion mass gets heavier as pressure increases.

Ion fluxes and energies will change significantly with pressure in this collisional sheath.
Specific conclusions:

- SiBr1,2 molecular data is critical in the correct understanding of this etch process.
- SiBr1,2 ions are important in determining the etch profile and have pressure dependant concentrations (and therefore fluxes and energies).
- Cross-sections with SiBr4 and SiBr3 could be included.
  - SiBr3,4 are not expected to be important etch products
  - Ions of SiBr3,4 could be important however.

General conclusions:

- The availability of molecular data is critical to understanding the gas-phase.
  - ...and therefore what arrives at the surface.
- Cross-sections can and have been calculated on demand for these applications.
Thank you for listening

Brought to you by:

Dr. James Munro

Prof. Jonathan Tennyson, Mr. Stephen Harrison

Dr. Song-Yun Kang

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Dr. Josef Brcka (for 2D Comsol model)
T. Mori, M. Sasaki, T. Nishizuka and T. Nozawa (for experiment)
Methane

![Methane molecular structure](image)

Diagram showing the total cross section (in Angstroms) as a function of electron energy (in eV) for various basis sets: 6-31G (SE), 6-31G (20 states, contracted), 6-31G (40 states, contracted), DZP (48 states, contracted), 6-31G (48 states, contracted), 6-31G (48 states, uncontracted). Data points from Lengsfeld et al. (1991), Lohmann and Buckman (1986), and Ferch et al. (1985) are also included.